

1-Octanol
111-87-5 | DTXSID7021940

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.99

Global applicability domain: Inside

Local applicability domain index: 7.35e-01

Confidence level: 8.09e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 3.00</div> <div>Predicted: 2.99</div>	<div>Image not found</div> <div>2-Octanol</div> <div>Measured: 2.90</div> <div>Predicted: 2.75</div>	<div>Image not found</div> <div>1-Nonanol</div> <div>Measured: 3.77</div> <div>Predicted: 3.72</div>
<div>Image not found</div> <div>1-Heptanol</div> <div>Measured: 2.62</div> <div>Predicted: 2.53</div>		